Low rank positive partial transpose states and their relation to product vectors

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Abstract

It is known that entangled mixed states that are positive under partial transposition (PPT states) must have rank at least four. In a previous paper we presented a classification of rank four entangled PPT states which we believe to be complete. In the present paper we continue our investigations of the low rank entangled PPT states. We use perturbation theory in order to construct rank five entangled PPT states close to the known rank four states, and in order to compute dimensions and study the geometry of surfaces of low rank PPT states. We exploit the close connection between low rank PPT states and product vectors. In particular, we show how to reconstruct a PPT state from a sufficient number of product vectors in its kernel. It may seem surprising that the number of product vectors needed may be smaller than the dimension of the kernel.

1 Introduction

Quantum entanglement between subsystems of a composite physical system is a phenomenon which clearly distinguishes quantum physics from classical physics [1]. Entangled quantum states show correlations between measurements on the subsystems which can not be modelled within classical physics with local interactions. A classical model would have to be a joint probability distribution of quantitities that are incompatible in the quantum theory, and the existence of such a joint probability distribution, consistent with locality, implies so called Bell inequalities [2], or even equalities as in the three particle states known as GHZ states, introduced by Mermin, Greenberger, Horne, and Zeilinger [3, 4]. The correlations in entangled quantum states violate Bell inequalities and GHZ equalities.

A pure classical state of a composite system has no correlations between measurements on subsystems, since classical measurements are deterministic. A statistical ensemble of pure classical states, what we may call a mixed classical state, can have correlations, but these correlations can not violate Bell inequalities, by definition.

The only pure quantum states that are not entangled are the pure product states, which resemble pure classical states in that they have no correlations at all. By definition, a mixed quantum state is a statistical ensemble of pure quantum states, and it is said to be separable if it can be mixed entirely from pure product states. The separable mixed states are not entangled, since they can not violate Bell inequalities. The entangled mixed states are precisely those that are non-separable. For this reason,

the mathematical distinction between separable and non-separable mixed states is important from the physical point of view.

The separability problem, how to characterize the set $\mathcal{S}$ of separable mixed states and decide whether a given mixed state is separable or not, is known to be a difficult mathematical problem [5]. It motivates our work presented here and in previous papers, although we have not studied so much the separable states directly as the larger class of mixed states called PPT states [6, 7, 8, 9].

The separable mixed states have the property that they remain positive after partial transposition, they are PPT states, for short. The set $\mathcal{P}$ of PPT states is in general larger than the set $\mathcal{S}$ of separable states, but the difference between the two sets is surprisingly small in low dimensions, and in the very lowest dimensions, 2×2, 2×3, and 3×2, there is no difference [10].

The condition of positive partial transpose is known as the Peres separability criterion [11]. It is a powerful separability test, especially in low dimensions where the difference between the two sets $\mathcal{P}$ and $\mathcal{S}$ is small. It can be used for example to prove that any pure quantum state is either entangled or a pure product state.

We study especially the lowest rank entangled PPT states, on the assumption that they are the easiest ones to understand. In the present paper we discuss in particular how to construct PPT states of rank 4 and 5 in 3×3 dimensions, and rank 6 in 4×4 dimensions. A central theme is how the states are constrained by the existence of product vectors in the kernel. Another central theme is perturbation theory, which we use to contruct rank 5 PPT states close to rank 4 states, and to study surfaces of PPT states of fixed low rank. We compute numerically the dimensions of such surfaces, and we show how to follow a surface by numerical integration of an equation of motion.

The relation between PPT states and product vectors

The close connection between PPT states and product vectors has been used earlier, for example to prove the separability of sufficiently low rank PPT states [12].

Bennett et al. [13, 14] introduced a method for constructing low rank mixed states that are obviously entangled PPT states, using what they called Unextendible Product Bases (UPBs). From a UPB, defined as a maximal set of orthogonal product vectors which is not a complete basis of the Hilbert space, one constructs an orthogonal projection Q and the complementary projection $P = \mathbb{1} - Q$. Then $\rho = P/(\mathrm{Tr}\, P)$ is an entangled PPT state.

The UPB construction is most successful in the special case of rank 4 PPT states in 3×3 dimensions. In Ref. [9] we argued, partly based on evidence from numerical studies, that an extended version of the UPB construction, including nonunitary but nonsingular product transformations on the states, is general enough to produce all rank 4 entangled PPT states in 3×3 dimensions.

Unfortunately, attempts to apply the UPB method directly in higher dimensions fail, even when the kernel contains product vectors, because there can not exist a sufficient number of orthogonal product vectors. The orthogonality is essential in the construction by Bennett et al. of the PPT state as a projection operator. We would like to generalize the construction in such a way that it works without the orthogonality condition.

One possible generalization is to construct projection operators as more general convex combinations, or even as non-convex linear combinations, of pure product states. This idea is explored in a separate paper [15].

In the present paper we discuss in general the constraints imposed on a PPT state ρ by the existence of product vectors in its kernel, and we show that these constraints are so strong that they actually determine the state uniquely. A surprising discovery is that in cases where the kernel contains a finite overcomplete set of product vectors, the state ρ can be reconstructed from only a subset of the product

vectors, and the number of product vectors needed may even be smaller than the dimension of the kernel.

From this point of view, the important question is exactly what conditions the product vectors must satisfy in order for the constraint equations to have a solution for ρ. We can answer this question in the familiar special case of rank 4 PPT states in 3×3 dimensions, but not in other cases. We consider this an interesting problem for future research.

Outline of the paper

The contents of the present paper are organized as follows. First we review some linear algebra, in particular degenerate perturbation theory, in Sections 2, 3, and 4. The main purpose is to introduce notation and collect formulas for later reference.

In Section 5 we discuss the rank 4 PPT states in 3×3 dimensions. We review the UPB construction, based on orthogonal product vectors in the kernel, before we describe an approach which is different in that the product vectors need not be orthogonal. The new approach also throws some new light on a set of reality conditions that limit the selection of product vectors to be used for constructing rank 4 PPT states.

In Section 6 we discuss the rank 5 PPT states in 3×3 dimensions. We find an 8 dimensional surface of rank 5 PPT states in every generic 5 dimensional subspace, but we have not found any general method to construct such states. However, we show how to construct rank 5 PPT states by perturbing rank 4 PPT states. Again, the product vectors in the kernel of the rank 4 state play an important role in our construction of the rank 5 states.

In Section 7 we discuss rank 6 PPT states in 4×4 dimensions. The kernel of such a state has dimension 10, and contains 20 product vectors. The remarkable result we find is that the state can be constructed from only 7 product vectors in the kernel. An arbitrary set of 7 product vectors does not produce a rank 6 PPT state, but we do not know how to select sets of product vectors that can be used in such a construction.

In Section 8 we discuss briefly how to determine numerically the dimensions of surfaces of PPT states of fixed rank. We find that the dimensions are given by a simple counting of independent constraints, except for the very lowest rank states, for which the constraints are not independent.

Finally, we discuss in Section 9 how to study a surface of PPT states by numerical integration of equations of motion for curves on the surface. In this way one may study for example the curvature of the surface, or how a curve on the surface approaches the boundary of the surface.

2 Some basic linear algebra

2.1 Density matrices

Let H_N be the set of Hermitean $N \times N$ matrices. It has a natural structure as a real Hilbert space of dimension N^2 with the scalar product

$$(X, Y) = \mathrm{Tr}(XY) \ . \tag{1}$$

A mixed state, or density matrix, is a positive Hermitean matrix of unit trace. We define

$$\mathcal{D} = \mathcal{D}_N = \{ \, \rho \in H_N \mid \rho \geq 0 \, , \; \mathrm{Tr}\, \rho = 1 \, \} \ . \tag{2}$$

Because it is Hermitean, a density matrix ρ has a spectral representation in terms of a complete set of orthonormal eigenvectors $\psi_i \in \mathbb{C}^N$ with real eigenvalues λ_i,

$$\rho = \sum_{i=1}^{N} \lambda_i \, \psi_i \psi_i^\dagger \qquad \text{with} \qquad \psi_i^\dagger \psi_j = \delta_{ij} \;, \qquad \mathbb{1} = \sum_{i=1}^{N} \psi_i \psi_i^\dagger \;. \tag{3}$$

The rank of ρ is the number of eigenvalues $\lambda_i \neq 0$. The pseudoinverse of ρ is defined as

$$\rho^+ = \sum_{i, \lambda_i \neq 0} {\lambda_i}^{-1} \, \psi_i \psi_i^\dagger \;, \tag{4}$$

it is equal to the inverse ρ^{-1} if ρ is invertible. The matrices

$$P = \rho^+ \rho = \rho \rho^+ = \sum_{i, \lambda_i \neq 0} \psi_i \psi_i^\dagger \;, \qquad Q = \mathbb{1} - P = \sum_{i, \lambda_i = 0} \psi_i \psi_i^\dagger \tag{5}$$

are Hermitean and project orthogonally onto two complementary orthogonal subspaces of $\mathbb{C}^N$, P onto $\text{Img}\,\rho$, the image of ρ, and Q onto $\text{Ker}\,\rho$, the kernel of ρ. The relations $P\rho = \rho P = P\rho P = \rho$ and $Q\rho = \rho Q = Q\rho Q = 0$ will be used in the following.

We say that ρ is positive, or positive semidefinite, and we write $\rho \geq 0$, when $\lambda_i \geq 0$ for $i = 1, 2, \ldots, N$. An equivalent condition is that $\psi^\dagger \rho \psi \geq 0$ for all $\psi \in \mathbb{C}^N$. It follows from the last inequality and the spectral representation of ρ that $\psi^\dagger \rho \psi = 0$ if and only if $\rho\psi = 0$.

The definition of positive Hermitean matrices by inequalities of the form $\psi^\dagger \rho \psi \geq 0$ implies that $\mathcal{D}$ is a convex set. That is, if ρ is a convex combination of $\rho_1, \rho_2 \in \mathcal{D}$,

$$\rho = \lambda \rho_1 + (1 - \lambda) \rho_2 \qquad \text{with} \qquad 0 < \lambda < 1 \;, \tag{6}$$

then $\rho \in \mathcal{D}$. Furthermore, since $\text{Ker}\,\rho = \{\psi \mid \psi^\dagger \rho \psi = 0\}$ when $\rho \geq 0$, it follows that

$$\text{Ker}\,\rho = \text{Ker}\,\rho_1 \cap \text{Ker}\,\rho_2 \;, \tag{7}$$

independent of λ, when ρ is a convex combination as above. Since $\text{Ker}\,\rho$ is independent of λ, so is $\text{Img}\,\rho = (\text{Ker}\,\rho)^\perp$.

A convex set is defined by its extremal points: those points that are not convex combinations of other points. The extremal points of $\mathcal{D}$ are the pure states of the form $\rho = \psi\psi^\dagger$ with $\psi \in \mathbb{C}^N$. Thus, the spectral representation in eq. (3) is an expansion of ρ as a convex combination of N or fewer extremal points of $\mathcal{D}$.

Finite perturbations

In the following, let ρ be a density matrix and define the projections P and $Q = \mathbb{1} - P$ as in eq. (5). Consider a perturbation

$$\rho' = \rho + \epsilon A \;, \tag{8}$$

where $A \neq 0$ is Hermitean, and $\text{Tr}\,A = 0$ so that $\text{Tr}\,\rho' = \text{Tr}\,\rho$. The real parameter ϵ may be finite or infinitesimal, we will first consider the case when ϵ is finite.

We observe that if $\text{Img}\,A \subset \text{Img}\,\rho$, or equivalently if $PAP = A$, then there will be a finite range of values of ϵ, say $\epsilon_1 \leq \epsilon \leq \epsilon_2$ with $\epsilon_1 < 0 < \epsilon_2$, such that $\rho' \in \mathcal{D}$ and $\text{Img}\,\rho' = \text{Img}\,\rho$. This is so because the eigenvectors of ρ with zero eigenvalue will remain eigenvectors of ρ' with zero

eigenvalue, and all the positive eigenvalues of ρ will change continuously with ϵ into eigenvalues of ρ'.

The other way around, if $\rho' \in \mathcal{D}$ for $\epsilon_1 \leq \epsilon \leq \epsilon_2$ with $\epsilon_1 < 0 < \epsilon_2$, then ρ' is a convex combination of $\rho + \epsilon_1 A$ and $\rho + \epsilon_2 A$ for every ϵ in the open interval $\epsilon_1 < \epsilon < \epsilon_2$. Hence $\mathrm{Img}\,\rho'$ is independent of ϵ in this interval, implying that $\mathrm{Img}\,A \subset \mathrm{Img}\,\rho$ and $PAP = A$.

This shows that ρ is extremal in $\mathcal{D}$ if and only if there exists no $A \neq 0$ with $\mathrm{Tr}\,A = 0$ and $PAP = A$. Another formulation of the condition is that there exists no $\rho' \in \mathcal{D}$ with $\rho' \neq \rho$ and $\mathrm{Img}\,\rho' = \mathrm{Img}\,\rho$. A third equivalent formulation of the extremality condition is that the equation

$$PAP = A \tag{9}$$

for the Hermitean matrix A has $A = \rho$ as its only solution (up to proportionality). In fact, if $PBP = B$ and $\mathrm{Tr}\,B \neq 0$, then we have $PAP = A$ and $\mathrm{Tr}\,A = 0$ when we take

$$A = B - (\mathrm{Tr}\,B)\,\rho\ . \tag{10}$$

Infinitesimal perturbations

Assume now that $\mathrm{Img}\,A \not\subset \mathrm{Img}\,\rho$. The question is how an infinitesimal perturbation affects the zero eigenvalues of ρ. When ρ is of low rank we need degenerate perturbation theory, which is well known from any textbook on quantum mechanics.

To first order in ϵ, the zero eigenvalues of ρ are perturbed into eigenvalues of ρ' that are ϵ times the eigenvalues of QAQ on the subspace $\mathrm{Ker}\,\rho$. Similarly, to first order in ϵ, the positive eigenvalues of ρ are perturbed into positive eigenvalues of ρ', in a way which is determined by how ρ and PAP act on $\mathrm{Img}\,\rho$.

It is clear from this that, to first order in ϵ, the condition

$$QAQ = 0 \tag{11}$$

is necessary and sufficient to ensure that the rank of ρ' equals the rank of ρ, and that $\rho' \geq 0$ both for $\epsilon > 0$ and for $\epsilon < 0$.

More generally, to first order in ϵ, the rank of ρ' equals the rank of ρ plus the rank of QAQ. For example, if we want to perturb ρ in such a way that the rank increases by one, then we have to choose A such that

$$QAQ = \alpha\,\phi\phi^\dagger\ , \tag{12}$$

where $\phi \in \mathrm{Ker}\,\rho$ is a normalized eigenvector of QAQ with $\alpha \neq 0$ as eigenvalue. Since QAQ is Hermitean, α must be real. If $\alpha > 0$, then $\rho' \geq 0$ for $\epsilon > 0$ but not for $\epsilon < 0$.

Projection operators on H_N

Using the projections P and Q defined above we define projection operators on H_N, the real Hilbert space of Hermitean $N \times N$ matrices, as follows,

$$\begin{aligned} \mathbf{P}X &= PXP\ , \\ \mathbf{Q}X &= QXQ = X - PX - XP + PXP\ , \\ \mathbf{R}X &= (\mathbf{I} - \mathbf{P} - \mathbf{Q})X = PX + XP - 2PXP\ . \end{aligned} \tag{13}$$

Here $\mathbf{I}$ is the identity on H_N. It is straightforward to verify that these are complementary projections, with $\mathbf{P}^2 = \mathbf{P}$, $\mathbf{Q}^2 = \mathbf{Q}$, $\mathbf{PQ} = \mathbf{QP} = \mathbf{0}$, and so on. They are symmetric with respect to the natural scalar product on H_N, for example,

$$(X, \mathbf{P}Y) = \mathrm{Tr}(XPYP) = \mathrm{Tr}(PXPY) = (\mathbf{P}X, Y) \ . \tag{14}$$

Hence they project orthogonally, and relative to an orthonormal basis of H_N they are represented by symmetric matrices.

Relative to an orthonormal basis of $\mathbb{C}^N$ with the first basis vectors in $\mathrm{Img}\,\rho$ and the last basis vectors in $\mathrm{Ker}\,\rho$, a Hermitean matrix X takes the block form

$$X = \begin{pmatrix} U & V \\ V^\dagger & W \end{pmatrix} , \tag{15}$$

with $U^\dagger = U$ and $W^\dagger = W$. In this basis we have

$$P = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} , \qquad Q = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} , \tag{16}$$

and hence,

$$\mathbf{P}X = \begin{pmatrix} U & 0 \\ 0 & 0 \end{pmatrix} , \qquad \mathbf{Q}X = \begin{pmatrix} 0 & 0 \\ 0 & W \end{pmatrix} , \qquad \mathbf{R}X = \begin{pmatrix} 0 & V \\ V^\dagger & 0 \end{pmatrix} . \tag{17}$$

2.2 Composite systems

Product vectors

If $N = N_A N_B$ then the tensor product spaces $\mathbb{C}^N = \mathbb{C}^{N_A} \otimes \mathbb{C}^{N_B}$ (a complex tensor product) and $H_N = H_{N_A} \otimes H_{N_B}$ (a real tensor product) may describe a composite quantum system with two subsystems A and B of Hilbert space dimensions N_A and N_B.

A vector $\psi \in \mathbb{C}^N$ then has components $\psi_I = \psi_{ij}$, where

$$I = 1, 2, \ldots, N \quad \leftrightarrow \quad ij = 11, 12, \ldots, 1N_B, 21, 22, \ldots, N_A N_B \ . \tag{18}$$

A product vector $\psi = \phi \otimes \chi$ has components $\psi_{ij} = \phi_i \chi_j$. We see that ψ is a product vector if and only if its components satisfy the quadratic equations

$$\psi_{ij}\psi_{kl} - \psi_{il}\psi_{kj} = 0 \ . \tag{19}$$

These equations are not all independent, the number of independent complex equations is

$$K = (N_A - 1)(N_B - 1) = N - N_A - N_B + 1 \ . \tag{20}$$

For example, if $\psi_{11} \neq 0$ we get a complete set of independent equations by taking $i = j = 1$ and $k = 2, 3, \ldots, N_A$, $l = 2, 3, \ldots, N_B$.

Since the equations are homogeneous, any solution $\psi \neq 0$ gives rise to a one parameter family of solutions $c\psi$ with $c \in \mathbb{C}$. A vector ψ in a subspace of dimension n has n independent complex components. Since the most general nonzero solution must contain at least one free complex parameter, we conclude that a generic subspace of dimension n will contain nonzero product vectors if and only if

$$n \geq K + 1 = N - N_A - N_B + 2 \ . \tag{21}$$

The limiting dimension

$$n = N - N_A - N_B + 2 \tag{22}$$

is particularly interesting. In this special case a nonzero solution will contain exactly one free parameter, which has to be a complex normalization constant.

Thus, up to proportionality there will exist a finite set of product vectors in a generic subspace of dimension $n = N - N_A - N_B + 2$. The number of product vectors is [8]

$$p = \binom{N_A + N_B - 2}{N_A - 1} = \frac{(N_A + N_B - 2)!}{(N_A - 1)!\,(N_B - 1)!} \ . \tag{23}$$

A generic subspace of lower dimension will contain no nonzero product vector, whereas any subspace of higher dimension will contain a continuous infinity of different product vectors (different in the sense that they are not proportional).

Partial transposition

The following relation between matrix elements,

$$(X^P)_{ij;kl} = X_{il;kj} \ , \tag{24}$$

defines X^P, the partial transpose of the Hermitean matrix X with respect to the second subsystem.

A density matrix ρ is called separable if it is a convex combination of tensor product matrices,

$$\rho = \sum_k p_k \, \sigma_k \otimes \tau_k \ , \tag{25}$$

with $\sigma_k \in \mathcal{D}_{N_A}$, $\tau_k \in \mathcal{D}_{N_B}$, $p_k > 0$, $\sum_k p_k = 1$. We denote by $\mathcal{S}$ the set of separable matrices.

The partial transpose of the above separable matrix is

$$\rho^P = \sum_k p_k \, \sigma_k \otimes (\tau_k)^T \geq 0 \ . \tag{26}$$

The positivity of ρ^P is known as the Peres criterion, it is an easily testable necessary condition for separability. For this reason it is of interest to study the set of PPT (Positive Partial Transpose) matrices, defined as

$$\mathcal{P} = \{\, \rho \in \mathcal{D} \mid \rho^P \geq 0 \,\} = \mathcal{D} \cap \mathcal{D}^P \ . \tag{27}$$

We may call it the Peres set. A well known result is that $\mathcal{P} = \mathcal{S}$ for $N = N_A N_B \leq 6$, whereas $\mathcal{P}$ is strictly larger than $\mathcal{S}$ in higher dimensions [10].

We will classify low rank PPT states by the ranks (m, n) of ρ and ρ^P, respectively. Note that ranks (m, n) and (n, m) are equivalent for the purpose of classification, because of the symmetric roles of ρ and ρ^P.

Product transformations

A product transformation of the form

$$\rho \mapsto \rho' = aV\rho V^{\dagger} \qquad \text{with} \qquad V = V_A \otimes V_B \ , \tag{28}$$

where a is a normalization factor and $V_A \in \mathrm{SL}(N_A, \mathbb{C})$, $V_B \in \mathrm{SL}(N_B, \mathbb{C})$, preserves positivity, rank, separability, and other interesting properties that the density matrix ρ may have. For example, it preserves positivity of the partial transpose, because

$$(\rho')^P = a\widetilde{V}\rho^P\widetilde{V}^{\dagger} \qquad \text{with} \qquad \widetilde{V} = V_A \otimes V_B^* \ . \tag{29}$$

The image and kernel of ρ and ρ^P transform in the following ways,

$$\mathrm{Img}\,\rho' = V\,\mathrm{Img}\,\rho \ , \qquad \mathrm{Ker}\,\rho' = (V^{\dagger})^{-1}\,\mathrm{Ker}\,\rho \ , \tag{30}$$

and

$$\mathrm{Img}\,(\rho')^P = \widetilde{V}\,\mathrm{Img}\,\rho^P \ , \qquad \mathrm{Ker}\,(\rho')^P = (\widetilde{V}^{\dagger})^{-1}\,\mathrm{Ker}\,\rho^P \ . \tag{31}$$

All these transformations are of product form and hence preserve the number of product vectors in a subspace.

We say that two density matrices ρ and ρ' related in this way are SL $\otimes$ SL equivalent, or simply SL equivalent. The concept of SL equivalence is important to us here because it simplifies very much our efforts to classify the low rank PPT states.

3 Restricted perturbations

We have seen that eq. (9) ensures that the perturbation $\rho' = \rho + \epsilon A$ preserves the image of ρ, so that $\mathrm{Img}\,\rho' = \mathrm{Img}\,\rho$ for infinitesimal values of the perturbation parameter ϵ, and $\mathrm{Img}\,\rho' \subset \mathrm{Img}\,\rho$ even for finite values of ϵ. The weaker condition in eq. (11) ensures only that the rank of ρ' equals the rank of ρ for infinitesimal values of ϵ.

We want to discuss how to use perturbations with similar restrictions in order to study, for example, the extremal points of the convex set $\mathcal{P}$. In particular, we are interested in perturbations that either preserve the ranks (m, n) of ρ, or else change these ranks in controlled ways.

In a similar way as we did for ρ, we define $\widetilde{P}$ and $\widetilde{Q} = \mathbb{1} - \widetilde{P}$ as the orthogonal projections onto $\mathrm{Img}\,\rho^P$ and $\mathrm{Ker}\,\rho^P$. Then we define

$$\begin{aligned}
\widetilde{\mathbf{P}}X &= (\widetilde{P}X^P\widetilde{P})^P \ , \\
\widetilde{\mathbf{Q}}X &= (\widetilde{Q}X^P\widetilde{Q})^P = X - (\widetilde{P}X^P)^P - (X^P\widetilde{P})^P + (\widetilde{P}X^P\widetilde{P})^P \ , \\
\widetilde{\mathbf{R}}X &= (\mathbf{I} - \widetilde{\mathbf{P}} - \widetilde{\mathbf{Q}})X = (\widetilde{P}X^P)^P + (X^P\widetilde{P})^P - 2(\widetilde{P}X^P\widetilde{P})^P \ .
\end{aligned} \tag{32}$$

These are again projections on the real Hilbert space H_N, like $\mathbf{P}$, $\mathbf{Q}$ and $\mathbf{R}$, again symmetric with respect to the natural scalar product on H_N.

We may now use the projection operators on H_N to impose various restrictions on the perturbation matrix A.

Testing for extremality in $\mathcal{P}$

The extremality condition for $\mathcal{P}$ is derived in a similar way as the extremality condition for $\mathcal{D}$ based on eq. (9). Clearly ρ is extremal in $\mathcal{P}$ if and only if there exists no $\rho' \in \mathcal{P}$, $\rho' \neq \rho$, with both $\operatorname{Img}\rho' = \operatorname{Img}\rho$ and $\operatorname{Img}(\rho')^P = \operatorname{Img}\rho^P$. Another way to formulate this condition is that $A = \rho$ is the only solution of the two equations $\mathbf{P}A = A$ and $\widetilde{\mathbf{P}}A = A$.

Since $\mathbf{P}$ and $\widetilde{\mathbf{P}}$ are projections, the equations $\mathbf{P}A = A$ and $\widetilde{\mathbf{P}}A = A$ together are equivalent to the single eigenvalue equation

$$(\mathbf{P} + \widetilde{\mathbf{P}})A = 2A\ . \tag{33}$$

They are also equivalent to either one of the eigenvalue equations

$$\mathbf{P}\widetilde{\mathbf{P}}\mathbf{P}A = A\ , \qquad \widetilde{\mathbf{P}}\mathbf{P}\widetilde{\mathbf{P}}A = A\ . \tag{34}$$

Note that the operators $\mathbf{P} + \widetilde{\mathbf{P}}$, $\mathbf{P}\widetilde{\mathbf{P}}\mathbf{P}$, and $\widetilde{\mathbf{P}}\mathbf{P}\widetilde{\mathbf{P}}$ are all real symmetric and therefore have complete sets of real eigenvalues and eigenvectors. In fact, the eigenvalues are all non-negative, because the operators are positive semidefinite.

When we diagonalize $\mathbf{P} + \widetilde{\mathbf{P}}$ we will always find $A = \rho$ as an eigenvector with eigenvalue 2. If it is the only solution of eq. (33), this proves that ρ is extremal in $\mathcal{P}$. If A is a solution not proportional to ρ, then we may impose the condition $\operatorname{Tr} A = 0$ (replace A by $A - (\operatorname{Tr} A)\rho$ if necessary), and we know that there exists a finite range of both positive and negative values of ϵ such that $\rho' = \rho + \epsilon A \in \mathcal{P}$, hence ρ is not extremal.

It should be noted that in our numerical calculations we may find eigenvalues of $\mathbf{P} + \widetilde{\mathbf{P}}$ that differ from 2 by less than one per cent. However, since eigenvalues are calculated with a precision close to the internal precision of the computer, which is of order 10^{-16}, there is never any ambiguity as to whether an eigenvalue is equal to 2 or strictly smaller than 2.

Perturbations preserving the PPT property and ranks

The rank and positivity of ρ is preserved by the perturbation, to first order in ϵ, both for $\epsilon > 0$ and $\epsilon < 0$, if and only if $\mathbf{Q}A = 0$. Similarly, the rank and positivity of ρ^P is preserved if and only if $\widetilde{\mathbf{Q}}A = 0$. These two equations together are equivalent to the single eigenvalue equation

$$(\mathbf{Q} + \widetilde{\mathbf{Q}})A = 0\ . \tag{35}$$

Again $\mathbf{Q} + \widetilde{\mathbf{Q}}$ is real symmetric and has a complete set of real eigenvalues and eigenvectors.

In conclusion, the perturbations that preserve the PPT property, as well as the ranks (m, n) of ρ and ρ^P, to first order in ϵ, are the solutions of eq. (35).

We may want to perturb in different ways, for example such that $\operatorname{Img}\rho' = \operatorname{Img}\rho$, but not necessarily $\operatorname{Img}(\rho')^P = \operatorname{Img}\rho^P$, we only require $(\rho')^P$ and ρ^P to have the same rank. Then the conditions on A are that $\mathbf{P}A = A$ and $\widetilde{\mathbf{Q}}A = 0$, or equivalently,

$$(\mathbf{I} - \mathbf{P} + \widetilde{\mathbf{Q}})A = 0\ . \tag{36}$$

4 Product vectors in the kernel

Assume that $\rho \in \mathcal{P}$. Recall that the equations $w^\dagger \rho w = 0$ and $\rho w = 0$ for $w \in \mathbb{C}^N$ are equivalent, and so are the equations $w^\dagger \rho^P w = 0$ and $\rho^P w = 0$, because $\rho \geq 0$ and $\rho^P \geq 0$. Taken together with the

identity

$$(x \otimes y)^\dagger \rho \, (u \otimes v) = (x \otimes v^*)^\dagger \rho^P (u \otimes y^*) \tag{37}$$

this puts strong restrictions on ρ when we know a number of product vectors in $\operatorname{Ker} \rho$.

Assume from now on that w is a product vector, $w = u \otimes v$. Defining $\widetilde{w} = u \otimes v^*$ we have the general relation

$$w^\dagger \rho w = \widetilde{w}^\dagger \rho^P \widetilde{w} \; . \tag{38}$$

Assume furthermore that $w \in \operatorname{Ker} \rho$, this is equivalent to the condition that $\widetilde{w} \in \operatorname{Ker} \rho^P$. For any $z \in \mathbb{C}^N$ we have the condition on ρ that $z^\dagger \rho w = 0$. In particular, when z is an arbitrary product vector, $z = x \otimes y$, we have the two conditions on ρ that

$$(x \otimes y)^\dagger \rho \, (u \otimes v) = 0 \tag{39}$$

and

$$(x \otimes v)^\dagger \rho \, (u \otimes y) = (x \otimes y^*)^\dagger \rho^P (u \otimes v^*) = 0 \; . \tag{40}$$

Assume that $w_i = u_i \otimes v_i \in \operatorname{Ker} \rho$ for $i = 1, 2, \ldots, n$. Then for arbitrary values of the indices i, j, k we have the following constraints on ρ,

$$(u_i \otimes v_j)^\dagger \rho \, (u_k \otimes v_k) = (u_i \otimes v_k)^\dagger \rho \, (u_k \otimes v_j) = 0 \; . \tag{41}$$

Let us introduce matrices

$$A_{klij} = (u_k \otimes v_l)(u_i \otimes v_j)^\dagger \; , \tag{42}$$

and Hermitean matrices

$$B_{klij} = A_{klij} + (A_{klij})^\dagger \; , \qquad C_{klij} = \mathrm{i} \, (A_{klij} - (A_{klij})^\dagger) \; , \tag{43}$$

then the constraints on ρ are of the form

$$\operatorname{Tr}(\rho B_{kkij}) = \operatorname{Tr}(\rho C_{kkij}) = \operatorname{Tr}(\rho B_{kjik}) = \operatorname{Tr}(\rho C_{kjik}) = 0 \; . \tag{44}$$

Each equation $\operatorname{Tr}(\rho B) = 0$ with $B \neq 0$ or $\operatorname{Tr}(\rho C) = 0$ with $C \neq 0$ is one real valued constraint. Of course, the constraints in eq. (44) are not all independent, we have for example that $C_{kkkk} = 0$.

5 Rank $(4, 4)$ PPT states in 3×3 dimensions

5.1 The UPB construction of entangled PPT states

We will review briefly the construction of a rank $(4, 4)$ entangled and extremal PPT state ρ in 3×3 dimensions from an unextendible orthonormal product basis (a UPB) of $\operatorname{Ker} \rho$ [13]. The UPB consists of five orthonormal product vectors $w_i = N_i u_i \otimes v_i$ with the property that there exists no product vector orthogonal to all of them. We include real normalization factors N_i here because we want to normalize such that $w_i^\dagger w_j = \delta_{ij}$ without necessarily normalizing the vectors u_i and v_i.

The orthogonality of the product vectors w_i follows from the orthogonality relations $u_1 \perp u_2 \perp u_3 \perp u_4 \perp u_5 \perp u_1$ and $v_1 \perp v_3 \perp v_5 \perp v_2 \perp v_4 \perp v_1$. There is the further condition that any three

vectors u_i and any three v_i are linearly independent. The five dimensional subspace spanned by these product vectors is the kernel of the density matrix

$$\rho = \frac{1}{4}\left(\mathbb{1} - \sum_{i=1}^{5} w_i w_i^\dagger\right) , \tag{45}$$

which is proportional to a projection operator. The partial transpose of ρ is

$$\rho^P = \frac{1}{4}\left(\mathbb{1} - \sum_{i=1}^{5} \widetilde{w}_i \widetilde{w}_i^\dagger\right) , \tag{46}$$

with $\widetilde{w}_i = N_i u_i \otimes v_i^*$. Thus we have both $\rho \geq 0$ and $\rho^P \geq 0$ by construction. Note that if all the vectors v_i are real, $v_i^* = v_i$, then ρ is symmetric under partial transposition, $\rho^P = \rho$.

By a unitary product transformation as in eq. (30) we may transform the above orthogonal UPB into the standard unnormalized form [9]

$$u = \begin{pmatrix} 1 & 0 & a & b & 0 \\ 0 & 1 & 0 & 1 & a \\ 0 & 0 & b & -a & 1 \end{pmatrix} , \qquad v = \begin{pmatrix} 1 & d & 0 & 0 & c \\ 0 & 1 & 1 & c & 0 \\ 0 & -c & 0 & 1 & d \end{pmatrix} , \tag{47}$$

with a, b, c, d as positive real parameters. The following quantities determine these parameters,

$$\begin{aligned} s_1 &= -\frac{\det(u_1u_2u_4)\ \det(u_1u_3u_5)}{\det(u_1u_2u_5)\ \det(u_1u_3u_4)} = a^2 , \\ s_2 &= -\frac{\det(u_1u_2u_3)\ \det(u_2u_4u_5)}{\det(u_1u_2u_4)\ \det(u_2u_3u_5)} = \frac{b^2}{a^2} , \end{aligned} \tag{48}$$

and

$$\begin{aligned} s_3 &= \frac{\det(v_1v_2v_3)\ \det(v_1v_4v_5)}{\det(v_1v_2v_5)\ \det(v_1v_3v_4)} = c^2 , \\ s_4 &= \frac{\det(v_1v_3v_5)\ \det(v_2v_3v_4)}{\det(v_1v_2v_3)\ \det(v_3v_4v_5)} = \frac{d^2}{c^2} . \end{aligned} \tag{49}$$

These ratios of determinants are invariant under general SL $\otimes$ SL transformations, as well as independent of the normalization of the vectors.

In Ref. [9] we presented numerical evidence that every entangled rank $(4, 4)$ PPT state is SL $\otimes$ SL equivalent to some state of the form of eq. (45) with real product vectors as given in eq. (47).

This means that the surface of all rank $(4, 4)$ entangled PPT states has dimension 36. We count 32 degrees of freedom due to the $\mathrm{SL}(3, \mathbb{C}) \otimes \mathrm{SL}(3, \mathbb{C})$ transformations, plus the 4 real SL $\otimes$ SL invariant parameters a, b, c, d in eq. (47).

5.2 A different point of view

We will present here the construction of an entangled PPT state ρ of rank $(4, 4)$ as seen from a different point of view. When ρ has rank 4 it means that $\mathrm{Ker}\,\rho$ has dimension 5. A generic 5 dimensional subspace in $\mathbb{C}^9 = \mathbb{C}^3 \otimes \mathbb{C}^3$ has a basis of product vectors. In fact, it contains exactly 6 product vectors, any 5 of which are linearly independent. By eq. (22), 5 is the limiting dimension for which the number of product vectors is nonzero and finite, and the number 6 is consistent with eq. (23).

Any set of 5 product vectors $w_i = u_i \otimes v_i$, orthogonal or not, may be transformed by an SL $\otimes$ SL transformation to the standard unnormalized form

$$u = \begin{pmatrix} 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & p \\ 0 & 0 & 1 & 1 & q \end{pmatrix} , \qquad v = \begin{pmatrix} 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & r \\ 0 & 0 & 1 & 1 & s \end{pmatrix} , \tag{50}$$

with p, q, r, s as real or complex parameters. We impose here again the condition that any three u_i and any three v_i should be linearly independent. There is always a 6th product vector which is a linear combination of the above 5,

$$u_6 = \begin{pmatrix} \frac{s-r}{ps-qr} \\ \frac{1-s}{q-s} \\ \frac{r-1}{r-p} \end{pmatrix} , \qquad v_6 = \begin{pmatrix} \frac{p-q}{ps-qr} \\ \frac{q-1}{q-s} \\ \frac{1-p}{r-p} \end{pmatrix} . \tag{51}$$

The values of the above invariants as functions of the new parameters are

$$s_1 = -\frac{p}{q} , \qquad s_2 = q - 1 , \qquad s_3 = \frac{r-s}{s} , \qquad s_4 = \frac{r}{1-r} . \tag{52}$$

The parameters p, q, r, s are actually new invariants, they can not be changed by SL $\otimes$ SL transformations.

If the values of p, q, r, s are such that the invariants s_1, s_2, s_3, s_4 are all real and strictly positive, then we may use eq. (48) and eq. (49) to find corresponding values of a, b, c, d, and we may transform from the non-orthogonal standard form in eq. (50) to the orthogonal standard form in eq. (47), which in turn defines the rank $(4, 4)$ state in eq. (45).

We see from eq. (52) that the invariants are all strictly positive if and only if p, q, r, s are all real, and $p < 0$, $q > 1$, $0 < r < 1$, $0 < s < r$. These inequalities define the regions marked 1 in the (p, q) and (r, s) planes as plotted in Fig. 1.

As discussed in ref. [9] there are 10 permutations of the product vectors w_i for $i = 1, 2, \ldots, 5$ which preserve the positivity of the invariants. These permutations form a group G which is the symmetry group of a regular pentagon, exemplified by the rotation, or cyclic permutation, $w_i \mapsto \widetilde{w}_i$ with

$$\widetilde{w}_1 = w_5 , \quad \widetilde{w}_2 = w_1 , \quad \widetilde{w}_3 = w_2 , \quad \widetilde{w}_4 = w_3 , \quad \widetilde{w}_5 = w_4 , \tag{53}$$

and the reflection

$$\widetilde{w}_1 = w_4 , \quad \widetilde{w}_2 = w_3 , \quad \widetilde{w}_3 = w_2 , \quad \widetilde{w}_4 = w_1 , \quad \widetilde{w}_5 = w_5 . \tag{54}$$

For short, we write the rotation as 51234 and the reflection as 43215.

There are altogether $5! = 120$ permutations of the 5 product vectors w_i, and they fall into 12 classes (left cosets of the group G as a subgroup of the permutation group S_5) which are not transformed into each other by G. We number the classes from 1 to 12, and pick one representative from each class as follows,

$$\begin{array}{llllll} 1: \ 12345 & 2: \ 13245 & 3: \ 21345 & 4: \ 23145 & 5: \ 31245 & 6: \ 32145 \\ 7: \ 12435 & 8: \ 14235 & 9: \ 21435 & 10: \ 24135 & 11: \ 13425 & 12: \ 14325 \end{array} \tag{55}$$

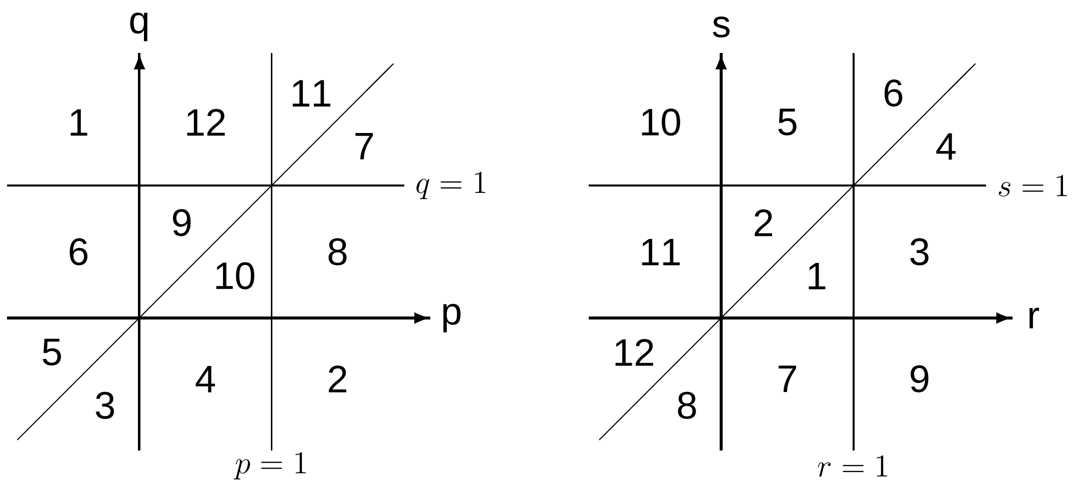

Figure 1: Regions for the parameters p, q, r, s defined in eq. (50) such that the product vectors $u_i \otimes v_i$ for $i = 1, 2, \ldots, 5$ are in the kernel of a rank $(4, 4)$ extremal PPT state. The (p, q) plane is divided into 12 regions, with 12 corresponding regions in the (r, s) plane. The numbers 1 to 12 refer to the permutations of product vectors given in eq. (55). For example, if (p, q) is in region 7, (r, s) must also be in region 7.

Each of these 12 classes defines a positivity region in each of the two parameter planes, where all 4 invariants $\widetilde{s}_1, \widetilde{s}_2, \widetilde{s}_3, \widetilde{s}_4$ computed from the permuted product vectors are positive. The 12 regions are disjoint and fill the planes completely, as shown in Fig. 1. On the border lines between the regions the condition of linear independence between any three u vectors and any three v vectors is violated.

To summarize, we have learned how to test whether a set of 5 product vectors $w_i = u_i \otimes v_i$, which is generic in the sense that any three u vectors are linearly independent and any three v vectors are also linearly independent, span the kernel of a rank $(4, 4)$ PPT state. We transform to the standard form defined in eq. (50), by a product transformation and normalization. Then the necessary and sufficient condition is that the parameters p, q, r, s are all real, and that the parameter pairs (p, q) and (r, s) lie in corresponding regions in the parameter planes, as shown in Figure 1.

It should be stressed that these conclusions are based in part on numerical evidence, and we have no analytical proof which is complete in every detail.

We will discuss next how to reconstruct a PPT state from the product vectors in its kernel.

5.3 Matrix representation relative to a non-orthonormal basis

Consider a basis $\{e_i\}$ consisting of vectors that need not be orthonormal. The scalar products

$$g_{ij} = e_i^\dagger e_j \tag{56}$$

define the metric tensor g as a Hermitean matrix. In the usual way, we write the inverse matrix g^{-1} with upper indices, so that

$$\sum_j g^{ij} g_{jk} = \delta^i_k \ . \tag{57}$$

We define the dual vectors e^j such that

$$e^i = \sum_j g^{ji} e_j \ , \qquad (e^i)^\dagger = \sum_j g^{ij} e_j^\dagger \ . \tag{58}$$

They satisfy the orthogonality relations

$$(e^i)^\dagger e_j = e_j^\dagger e^i = \delta^i_j \ , \tag{59}$$

and the completeness relation

$$\mathbb{1} = \sum_{i,j} e_i g^{ij} e_j^\dagger = \sum_j e^j e_j^\dagger = \sum_i e_i (e^i)^\dagger \ . \tag{60}$$

Using the dual basis vectors and the completeness relation we may write any matrix A as

$$A = \sum_{i,j} e^i \widetilde{A}_{ij} (e^j)^\dagger \qquad \text{with} \qquad \widetilde{A}_{ij} = e_i^\dagger A e_j \ . \tag{61}$$

5.4 Conditions on ρ from product vectors in Ker ρ

It is possible to construct the rank $(4,4)$ PPT state ρ directly from 5 product vectors in Ker ρ without transforming first the product vectors to the orthogonal form. We now describe this construction.

Given three product vectors $w_i = u_i \otimes v_i$ in Ker ρ, with the restriction that all three u_i and all three v_i are linearly independent. Then we have the following product basis of $\mathbb{C}^9$, not necessarily orthonormal,

$$e_{ij} = u_i \otimes v_j \ , \qquad ij = 11, 12, 13, 21, 22, 23, 31, 32, 33 \ . \tag{62}$$

With respect to this basis we may define matrix elements of ρ like in eq. (61),

$$\widetilde{\rho}_{ij;kl} = e_{ij}^\dagger \, \rho \, e_{kl} \ . \tag{63}$$

In order to count the independent constraints, it is convenient use the standard form of the product vectors defined in eq. (50). Now all the constraints from eq. (44) imply that

$$\widetilde{\rho} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & a_1 & b_1 & 0 & 0 & 0 & 0 & b_2 & 0 \\ 0 & b_1^* & a_2 & 0 & 0 & b_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & a_3 & 0 & b_4 & b_5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_3^* & b_4^* & 0 & a_4 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_5^* & 0 & 0 & a_5 & b_6 & 0 \\ 0 & b_2^* & 0 & 0 & 0 & 0 & b_6^* & a_6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} , \tag{64}$$

with real diagonal elements $a_1, a_2, \dots, a_6$ and complex off-diagonal elements $b_1, b_2, \dots, b_6$. This Hermitean 9×9 matrix contains 18 real parameters, which means that there are altogether $81 - 18 = 63$ independent real constraints.

Including the fourth product vector from eq. (50) gives additional constraints $\widetilde{\rho} w_4 = 0$, or explicitly written out,

$$\begin{aligned} a_1 + b_1 + b_2 &= 0 \ , \\ b_1^* + a_2 + b_3 &= 0 \ , \\ a_3 + b_4 + b_5 &= 0 \ , \\ b_3 + b_4 + a_4 &= 0 \ , \\ b_5^* + a_5 + b_6 &= 0 \ , \\ b_2 + b_6 + a_6 &= 0 \ . \end{aligned} \tag{65}$$

Here we have simplified slightly by complex conjugating the 4th and the 6th equation. These are complex equations, to be split into real and imaginary parts. The real parts are 6 independent equations, whereas the complex parts are only 5 independent equations. However, we get another independent equation as the imaginary part of, for example, the complex equation

$$(u_1 \otimes v_4)^\dagger \, \rho \, (u_4 \otimes v_2) = a_1 + b_1^* + b_2 = 0 \ . \tag{66}$$

The end result is that all the off-diagonal matrix elements b_i have to be real. Altogether, we get 12 independent real constraints, 6 from the real parts and 6 from the imaginary parts of the equations.

Thus, including the 4th product vector in $\mathrm{Ker}\,\rho$ increases the number of independent real constraints from 63 to 75, and reduces the number of real parameters in ρ from 18 to 6.

The generic case with 5 product vectors is that there are 81 independent constraints, leaving only the trivial solution $\rho = 0$. In order to end up with one possible solution for ρ we have to choose the parameters p, q, r, s to be real.

When we choose real values for p, q, r, s, there is always (generically) exactly one solution for ρ, that is, there are 80 independent constraints. The problem is that this uniquely determined matrix ρ, or its partial transpose, has in general both positive and negative eigenvalues.

The condition to ensure that both $\rho \geq 0$ and $\rho^P \geq 0$ (with the proper choice of sign for ρ), when the parameters p, q, r, s are real, is that the pair (p, q) and the pair (r, s) must lie in corresponding parameter regions, as shown in Fig. 1.

5.5 Separable states of rank $(4, 4)$

A separable state of rank 4 has the form

$$\rho = \sum_{i=1}^{4} \lambda_i \, \psi_i \psi_i^\dagger \ , \tag{67}$$

with $\lambda_i > 0$, $\sum_{i=1}^4 \lambda_i = 1$, $\psi_i^\dagger \psi_i = 1$, and $\psi_i = C_i \, \phi_i \otimes \chi_i$ with C_i as a normalization constant. In the generic case when any three vectors ϕ_i and any three χ_i are linearly independent, we may perform an SL $\otimes$ SL transformation and obtain the standard form

$$\phi = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix} , \qquad \chi = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix} . \tag{68}$$

In this standard form the χ vectors are real, and hence $\rho^P = \rho$.

The kernel $\operatorname{Ker}\rho$ consists of the vectors that are orthogonal to all 4 product vectors ψ_i, and it contains exactly 6 product vectors $w_i = N_i\, u_i \otimes v_i$, as follows,

$$u = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & -1 & 0 & 0 & -1 \\ 1 & 0 & 1 & 0 & -1 & 0 \end{pmatrix}, \qquad v = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 1 & 0 \\ 0 & -1 & 0 & -1 & 0 & 1 \end{pmatrix}. \tag{69}$$

Note that the product vectors in the kernel of a separable rank $(4,4)$ PPT state are not generic, in that there are subsets of three linearly dependent vectors both among the u vectors and among the v vectors.

The surface of separable states of rank 4 has dimension $35 = 32 + 3$, where 32 is the number of parameters of the group $\mathrm{SL}(3,\mathbb{C}) \otimes \mathrm{SL}(3,\mathbb{C})$ and 3 is the number of independent coefficients λ_i in eq. (67).

6 Rank $(5,5)$ PPT states in 3×3 dimensions

6.1 The surface of rank $(5,5)$ PPT states

Since we believe that we understand completely the rank $(4,4)$ entangled states in dimension 3×3, a natural next step is to try to understand the $(5,5)$ states in the same dimension.

As discussed in the previous section, a generic 5 dimensional subspace in 3×3 dimensions contains exactly 6 product vectors, which can be transformed by $\mathrm{SL}\otimes\mathrm{SL}$ transformations, as in eqs. (30) and (31), into the standard form given in eqs. (50) and (51), with SL$\otimes$SL invariant complex parameters p, q, r, s. Thus, each such subspace belongs to an equivalence class under $\mathrm{SL}\otimes\mathrm{SL}$ transformations, and the equivalence classes are parametrized by 8 real parameters. There is a discrete ambiguity in the parametrization, since it depends on the ordering of the 6 product vectors.

In one given generic 5 dimensional subspace we may construct a 5 dimensional set of rank $(5,5)$ separable states as convex combinations of the 6 product vectors in the subspace. However, we find numerically that the dimension of the surface of rank $(5,5)$ PPT states with the given subspace as image is not 5 but 8. We compute this dimension in the following way.

We search numerically for one rank $(5,5)$ state ρ, for example by the methods described in [8]. The state we find will typically be entangled and extremal in $\mathcal{P}$. From this state ρ we compute the projections $P, Q, \widetilde{P}, \widetilde{Q}$ as described in Sections 2 and 3, and we look for perturbations $\rho' = \rho + \epsilon A$, with $\operatorname{Tr} A = 0$, where A satifies both equations $\mathbf{P}A = PAP = A$ and $\widetilde{\mathbf{Q}}A = (\widetilde{Q}A^P\widetilde{Q})^P = 0$, or equivalently eq. (36),

$$(\mathbf{I} - \mathbf{P} + \widetilde{\mathbf{Q}})A = 0\ . \tag{70}$$

The number of linearly independent solutions for A is the dimension of the surface of rank $(5,5)$ PPT states at the point ρ.

We believe that the dimension 8 can be understood as follows. We may fix both subspaces $\operatorname{Img}\rho$ and $\operatorname{Img}\rho^P$, this means that we fix the projections P and $\widetilde{P}$ and determine ρ as a solution of the equation

$$(2\mathbf{I} - \mathbf{P} - \widetilde{\mathbf{P}})\rho = 0\ , \tag{71}$$

with $\operatorname{Tr}\rho = 1$. Then there is typically no solution at all for ρ, solutions exist only for special pairs of subspaces. If now the two 5 dimensional subspaces are chosen in such a way that a solution exists, then the solution is (typically) unique, and the uniqueness means that ρ is an extremal point of $\mathcal{P}$.

We may fix instead Img ρ but not Img ρ^P, only the rank of ρ^P. Then there is a set of solutions for ρ described by 8 real parameters. It is a natural guess that the role of these 8 parameters is to specify the SL $\otimes$ SL equivalence class to which the 5 dimensional subspace Img ρ^P belongs.

In fact, when we fix Img ρ there is no degree of freedom left corresponding to SL $\otimes$ SL transformations. This is so because the set of product vectors in Img ρ is discrete and can not be transformed continuously within the fixed subspace Img ρ. Hence, the only way to vary the subspace Img ρ^P without varying Img ρ is to vary the equivalence class of Img ρ^P.

Figure 2 shows a two dimensional section through the set of density matrices. The section is defined by the maximally mixed state, by a randomly selected rank $(5, 5)$ entangled and extremal PPT state ρ, and by a direction A through ρ such that the perturbed state $\rho' = \rho + \epsilon A$ is a rank $(5, 5)$ PPT state for infinitesimal positive and negative ϵ, and has Img $\rho' =$ Img ρ even for finite ϵ. The figure illustrates the fact that the difference between the sets $\mathcal{P}$ and $\mathcal{S}$ is small. It also illustrates that the difference between $\mathcal{P}$ and $\mathcal{S}$ is largest close to extremal entangled PPT states.

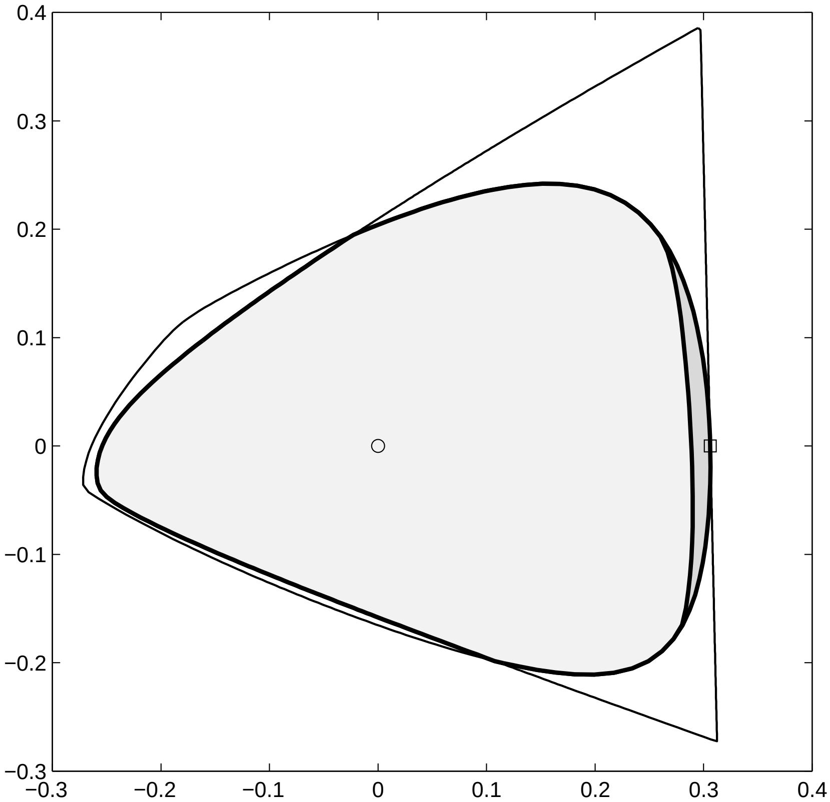

Figure 2: Two dimensional section through $\mathcal{D}$, the set of density matrices in 3×3 dimensions. The boundaries of $\mathcal{S}$, the set of separable states, and of $\mathcal{P}$, the set of PPT states, are both drawn as thick lines. The boundaries of $\mathcal{D}$ and of $\mathcal{D}^P$, the set of partially transposed density matrices, cross at two points, they are drawn as thin lines where they do not coincide with the boundary of $\mathcal{P}$. The origin, marked by a small circle, is the maximally mixed state. The point marked by a small square is an extremal rank $(5, 5)$ PPT state. The boundary of $\mathcal{D}$ is drawn through this point as a thin straight line. The boundary of $\mathcal{D}^P$ is drawn thick at this point, beacause it is also the boundary of $\mathcal{P}$. The lightly shaded region around the origin is $\mathcal{S}$. The small and more darkly shaded region close to the $(5, 5)$ state is the difference between $\mathcal{P}$ and $\mathcal{S}$. Away from this small region, the boundaries of $\mathcal{P}$ and $\mathcal{S}$ are indistinguishable in the plot.

If we want to allow both $\mathrm{Img}\,\rho$ and $\mathrm{Img}\,\rho^P$ to vary, but still require the ranks of ρ and ρ^P to be 5, the equation to be solved for the perturbation A is

$$(\mathbf{Q} + \widetilde{\mathbf{Q}})A = 0 \; . \tag{72}$$

In this case the number of linearly independent solutions for A is 48, and this is the dimension of the surface of all rank $(5, 5)$ PPT states.

We understand the dimension 48 as follows. There are $8 + 8 = 16$ parameters for the $\mathrm{SL} \otimes \mathrm{SL}$ equivalence classes of the subspaces $\mathrm{Img}\,\rho$ and $\mathrm{Img}\,\rho^P$. And there are 32 parameters for the $\mathrm{SL}(3, \mathbb{C}) \otimes \mathrm{SL}(3, \mathbb{C})$ transformations.

To summarize, an extremal (and hence entangled) rank $(5, 5)$ PPT state ρ is uniquely determined by eq. (71), as soon as we specify the 5 dimensional subspaces $\mathrm{Img}\,\rho$ and $\mathrm{Img}\,\rho^P$. Each subspace $\mathrm{Img}\,\rho$ and $\mathrm{Img}\,\rho^P$ is determined by 8 real $\mathrm{SL}\otimes\mathrm{SL}$ invariant parameters and an $\mathrm{SL}\otimes\mathrm{SL}$ transformation.

According to our understanding, based on numerical studies, which is so far only a plausible hypothesis, the 8 invariant parameters can be chosen independently for $\mathrm{Img}\,\rho$ and $\mathrm{Img}\,\rho^P$, but the $\mathrm{SL} \otimes \mathrm{SL}$ transformations can not be chosen independently. However, we do not know the relation that clearly exists between $\mathrm{Img}\,\rho$ and $\mathrm{Img}\,\rho^P$.

In other words, we do not know any explicit procedure for constructing the most general rank $(5, 5)$ PPT states. Therefore we turn next to a more restricted problem.

6.2 Perturbing from rank $(4, 4)$ to rank $(5, 5)$

We will see now how to construct $(5, 5)$ states that are infinitesimally close to $(4, 4)$ states.

Consider once more an infinitesimal perturbation $\rho' = \rho + \epsilon A$, this time with ρ as the rank $(4, 4)$ state defined in eq. (45), involving the standard real product vectors defined in eq. (47). The most general case is equivalent to this special case by some $\mathrm{SL} \otimes \mathrm{SL}$ transformation.

An extra bonus of this special choice of ρ is that $\rho^P = \rho$. In the notation we have used above, we have projections $P = \widetilde{P}$ on $\mathrm{Img}\,\rho = \mathrm{Img}\,\rho^P$ and $Q = \widetilde{Q}$ on $\mathrm{Ker}\,\rho = \mathrm{Ker}\,\rho^P$.

Conditions on the perturbation matrix A

By eq. (12), the condition for ρ' to have rank 5 is that

$$QAQ = \alpha\, ww^\dagger \; , \tag{73}$$

where α is a real number, $\alpha \neq 0$, and

$$w = \sum_{i=1}^{5} c_i w_i \; , \tag{74}$$

with complex coefficients c_i such that

$$w^\dagger w = \sum_{i=1}^{5} |c_i|^2 = 1 \; . \tag{75}$$

Similarly, the condition for $(\rho')^P$ to have rank 5 is that

$$\widetilde{Q} A^P \widetilde{Q} = QA^P Q = \beta\, zz^\dagger \; , \tag{76}$$

where β is real, $\beta \neq 0$, and

$$z = \sum_{i=1}^{5} d_i w_i \qquad \text{with} \qquad z^\dagger z = \sum_{i=1}^{5} |d_i|^2 = 1 \; . \tag{77}$$

Note that the possibilities that ρ' has rank either $(4,5)$ or $(5,4)$ are included if we allow either α or β to be zero.

By eq. (23), there is one extra product vector in Ker $\rho =$ Ker ρ^P, it may be written as

$$w_6 = \sum_{i=1}^{5} a_i w_i \; , \tag{78}$$

this time with real coefficients a_i. Since $w_i = N_i u_i \otimes v_i$ with N_i real and v_i real for $i = 1, 2, \ldots, 6$, we have for any Hermitean matrix A that

$$w_i^\dagger A w_i = w_i^\dagger A^P w_i \; . \tag{79}$$

By the definition of the projection Q we have that $Qw_i = w_i$ for $i = 1, 2, \ldots, 6$. It follows then from eq. (73) that

$$w_i^\dagger A w_i = w_i^\dagger Q A Q w_i = \alpha \, |w_i^\dagger w|^2 \; , \tag{80}$$

and from eq. (76) that

$$w_i^\dagger A^P w_i = w_i^\dagger Q A^P Q w_i = \beta \, |w_i^\dagger z|^2 \; . \tag{81}$$

Together with eq. (79) this gives the equations

$$\alpha \, |c_i|^2 = \beta \, |d_i|^2 \tag{82}$$

for $i = 1, 2, \ldots = 5$, and the 6th equation

$$\alpha \left| \sum_{i=1}^{5} a_i c_i \right|^2 = \beta \left| \sum_{i=1}^{5} a_i d_i \right|^2 \; . \tag{83}$$

It follows further that

$$\alpha = \sum_{i=1}^{5} \alpha \, |c_i|^2 = \sum_{i=1}^{5} \beta \, |d_i|^2 = \beta \; , \tag{84}$$

and that

$$|c_i| = |d_i| \qquad \text{for} \qquad i = 1, 2, \ldots, 5 \; . \tag{85}$$

Thus, the coefficient d_i can differ from c_i only by a phase factor. The total of 5 phase factors are reduced to 4 independent phase factors by the extra equation

$$\left| \sum_{i=1}^{5} a_i c_i \right| = \left| \sum_{i=1}^{5} a_i d_i \right| \; . \tag{86}$$

For infinitesimal values of ϵ, both ρ' and $(\rho')^P$ will have four eigenvalues infinitesimally close to $1/4$ and one eigenvalue close to zero, which is $\epsilon\alpha$ for ρ' and $\epsilon\beta$ for $(\rho')^P$. This eigenvalue is the same for ρ' and $(\rho')^P$, since $\alpha = \beta$. With $\alpha > 0$ this means that both $\rho' \geq 0$ and $(\rho')^P \geq 0$ for $\epsilon > 0$, but not for $\epsilon < 0$. Thus, we get automatically a PPT state of rank $(5,5)$, we never get rank $(5,4)$ or $(4,5)$. Also it never happens that ρ' is not a PPT state for the reason that one of ρ' or $(\rho')^P$ has a negative eigenvalue.

For a more general rank $(4,4)$ state ρ, which is obtained by some SL $\otimes$ SL transformation from a state of the special type discussed here, the smallest positive eigenvalues of ρ' and $(\rho')^P$ are no longer equal. But they are still tied together in such a way that they go to zero simultaneously when we move along the surface of $(5,5)$ states and approach its boundary. The boundary must therefore consist of $(4,4)$ states.

Computing A

Define $W = ww^\dagger$ and $Z = zz^\dagger$, in the same notation as above. These are both projections, $W^2 = W$ and $Z^2 = Z$, with $QW = WQ = W$ and $QZ = ZQ = Z$. It follows from eq. (73) and eq. (76) that

$$\begin{aligned} WAW &= WQAQW = \alpha W^3 = \alpha W = QAQ \;, \\ ZA^PZ &= ZQA^PQZ = \beta Z^3 = \beta Z = QA^PQ \;. \end{aligned} \tag{87}$$

Like in eq. (13) and eq. (32) we define

$$\mathbf{P}X = PXP \;, \quad \mathbf{Q}X = QXQ \;, \quad \widetilde{\mathbf{P}}X = (PX^PP)^P \;, \quad \widetilde{\mathbf{Q}}X = (QX^PQ)^P \;, \tag{88}$$

and furthermore,

$$\mathbf{W}X = WXW \;, \qquad \widetilde{\mathbf{Z}}X = (ZX^PZ)^P \;. \tag{89}$$

We may also define $\mathbf{S} = \mathbf{Q} - \mathbf{W}$ and $\widetilde{\mathbf{S}} = \widetilde{\mathbf{Q}} - \widetilde{\mathbf{Z}}$, these are again orthogonal projections on H_N.

The least restrictive conditions we may impose on A are now that both $\mathbf{S}A = 0$ and $\widetilde{\mathbf{S}}A = 0$, or equivalently,

$$(\mathbf{S} + \widetilde{\mathbf{S}})A = 0 \;. \tag{90}$$

To compute A from this equation we introduce an orthonormal basis in the real Hilbert space H_N. Relative to this basis, the operator $\mathbf{S} + \widetilde{\mathbf{S}}$ is represented by a real symmetric positive semidefinite matrix, which has a complete set of real eigenvectors with real eigenvalues. We choose A as an eigenvector of $\mathbf{S} + \widetilde{\mathbf{S}}$ with eigenvalue zero.

Apart from the trivial solution $A = \rho$, we find 37 linearly independent solutions of eq. (90). 36 out of these 37 are perturbations that give $\rho' = \rho + \epsilon A$ as a rank $(4,4)$ state both for $\epsilon > 0$ and $\epsilon < 0$. They do not depend on either vector w or z, since they satisfy the conditions $\mathbf{Q}A = 0$ and $\widetilde{\mathbf{Q}}A = 0$. But because $\mathbf{W} = \mathbf{WQ}$ and $\widetilde{\mathbf{Z}} = \widetilde{\mathbf{Z}}\widetilde{\mathbf{Q}}$ they also satisfy the conditions

$$\mathbf{W}A = \mathbf{WQ}A = 0 \;, \qquad \widetilde{\mathbf{Z}}A = \widetilde{\mathbf{Z}}\widetilde{\mathbf{Q}}A = 0 \;, \tag{91}$$

and hence eq. (90). The number 36 is the dimension of the surface of rank $(4,4)$ extremal PPT states, as noted in Subsection 5.1. The 37th independent solution is the one giving a rank $(5,5)$ extremal PPT state.

A more restricted class of perturbations consists of those where we fix the 5 dimensional subspace $\mathrm{Img}\,\rho'$ to be the direct sum of the 4 dimensional subspace $\mathrm{Img}\,\rho$ and the one dimensional subspace of the vector w. The projection on $\mathrm{Img}\,\rho'$ is then

$$P_5 = P + W \ , \tag{92}$$

and the partial condition on A is that $\mathbf{P}_5 A = A$, when we define

$$\mathbf{P}_5 X = P_5 X P_5 \ . \tag{93}$$

The full condition on A is that

$$(\mathbf{P}_5 - \widetilde{\mathbf{S}})A = A \ . \tag{94}$$

Again apart from the trivial solution $A = \rho$, we find 5 linearly independent solutions of eq. (94), of which 4 give ρ' as a rank $(4,4)$ state both for $\epsilon > 0$ and $\epsilon < 0$. The 5th independent solution is the one giving ρ' as a rank $(5,5)$ extremal PPT state.

The 4 directions that only give new $(4,4)$ states are easily identified, since they do not depend on the vector z. To find them we simply repeat the calculation with a "wrong" z, violating the conditions (85) and (86). In this way we find no $(5,5)$ state, but we find the same set of perturbations into $(4,4)$ states. The number 4 is the dimension of the surface of $(4,4)$ states with image within the fixed 5 dimensional subspace projected out by the projector P_5.

There is a natural explanation of why this surface has dimension 4. In fact, when we fix P_5 and look for $(4,4)$ states with image within this fixed 5 dimensional subspace, we eliminate all degrees of freedom corresponding to $\mathrm{SL} \otimes \mathrm{SL}$ transformations. But we still allow variations of the 4 real $\mathrm{SL} \otimes \mathrm{SL}$ invariant parameters that are needed to define a rank $(4,4)$ state.

We conclude that for fixed vectors w and z there is one direction away from the surface of rank $(4,4)$ extremal PPT states and into the surface of rank $(5,5)$ extremal PPT states.

For a fixed vector w there is a 4 parameter family of acceptable vectors z. Recall that these 4 parameters determine the 5 relative phases between the coefficients c_i in eq. (74) and the corresponding coefficients d_i in eq. (77).

The vector w is an arbitrary vector in the 5 dimensional kernel of the unperturbed state ρ, hence it contains 4 complex parameters, or 8 real parameters, after we take out an uninteresting complex normalization factor. Altogether, there are $8 + 4 = 12$ independent directions away from the 36 dimensional surface of rank $(4,4)$ PPT states and into the surface of rank $(5,5)$ PPT states.

When we perturb an arbitrary rank $(5,5)$ PPT state in such a way that we preserve the ranks of the state and its partial transpose, we find numerically that the surface of rank $(5,5)$ PPT states has dimension 48. The fact that $48 = 36 + 12$ is consistent with the hypothesis that we can reach every rank $(5,5)$ PPT state if we start from a rank $(4,4)$ PPT state and move continuously along the surface of rank $(5,5)$ PPT states.

7 Rank $(6,6)$ entangled PPT states in 4×4 dimensions

We will discuss in some detail one more example of the relation between PPT states and product vectors. According to eq. (22), the rank $(6,6)$ PPT states in 4×4 dimensions represent just the limiting case with a finite number of product vectors in the kernel, in this respect they are similar to the rank $(4,4)$ states in 3×3 dimensions.

The kernel of a rank 6 state in 16 dimensions has dimension 10, and the generic case, according to eq. (23), is that it contains exactly 20 product vectors, any 10 of which are linearly independent. We will see here that the product vectors in the kernel put such strong restrictions on the state that the rank $(6,6)$ PPT state may be reconstructed uniquely from only 7 product vectors in its kernel.

To see how it works, take a set of product vectors in 4×4 dimensions. We may take random product vectors, or else a set of product vectors with the special property that they belong to $\operatorname{Ker}\rho$ where ρ is a rank $(6,6)$ PPT state. We find numerically that the number of constraints generated by fewer than 7 product vectors is the same in both cases. We find the following numbers.

From 4 product vectors assumed to lie in $\operatorname{Ker}\rho$ for an unknown ρ, or actually lying in $\operatorname{Ker}\rho$ for a known ρ, we get 172 independent constraints on ρ of the form given in eq. (44). These constraints leave 84 free real parameters in ρ, before we normalize and set $\operatorname{Tr}\rho = 1$.

From 5 product vectors in $\operatorname{Ker}\rho$ we get 205 independent constraints, leaving 51 parameters in ρ.

From 6 product vectors in $\operatorname{Ker}\rho$ we get 234 independent constraints, and 22 parameters in ρ.

Finally, 7 product vectors in $\operatorname{Ker}\rho$ give either 255 or 256 independent constraints, and either 1 or 0 real parameters in ρ. If there is one parameter left, it is a proportionality constant, to be fixed by the normalization condition $\operatorname{Tr}\rho = 1$.

The standard form of 7 product vectors in 4×4 dimensions, generalizing eq. (50), is the following,

$$u = \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & p_1 & p_4 \\ 0 & 0 & 1 & 0 & 1 & p_2 & p_5 \\ 0 & 0 & 0 & 1 & 1 & p_3 & p_6 \end{pmatrix}, \qquad v = \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & p_7 & p_{10} \\ 0 & 0 & 1 & 0 & 1 & p_8 & p_{11} \\ 0 & 0 & 0 & 1 & 1 & p_9 & p_{12} \end{pmatrix}. \tag{95}$$

There are 12 complex parameters $p_1, p_2, \ldots, p_{12}$, that is, 24 real parameters. These are invariant in the sense that we can not change them by $\mathrm{SL}(4,\mathbb{C}) \otimes \mathrm{SL}(4,\mathbb{C})$ transformations.

Not just any arbitrary set of 7 product vectors defines a rank $(6,6)$ PPT state. We arrive at this conclusion not only because we find numerically that 7 generic product vectors allow only $\rho = 0$ as solution of all the constraint equations, but also because a dimension counting shows that we need less than 24 invariant parameters in order to parametrize the rank $(6,6)$ PPT states.

Take one known rank $(6,6)$ PPT state ρ and perturb it into another rank $(6,6)$ PPT state $\rho' = \rho + \epsilon A$ with ϵ infinitesimal. Here A must be a solution of eq. (35), with operators $\mathbf{Q}$ and $\widetilde{\mathbf{Q}}$ defined relative to ρ as explained. The number of linearly independent solutions for A, found numerically, is 76, including the trivial solution $A = \rho$. This shows that the surface of rank $(6,6)$ PPT states has 75 real dimensions.

Of these 75 dimensions, 60 dimensions result from product transformations $\rho \mapsto V\rho V^\dagger$ with $V = V_A \otimes V_B$ and $V_A, V_B \in \mathrm{SL}(4,\mathbb{C})$. The remaining 15 dimensions must correspond to 15 $\mathrm{SL}\otimes\mathrm{SL}$ invariant parameters of the 7 product vectors.

It is also worth noting that, by the counting explained in the next section, the set of 6 dimensional subspaces of $\mathbb{C}^{16}$ has real dimension $16^2 - 6^2 - 10^2 = 120$, much larger than the dimension 75 of the surface of $(6,6)$ states. Thus, not every 6 dimensional subspace of $\mathbb{C}^{16}$ is the host of a rank $(6,6)$ PPT state, as one would expect from the analogy to the case of the rank $(4,4)$ PPT states in $\mathbb{C}^9$.

8 Dimension counting

We will describe in this section how to compute numerically the dimensions of surfaces of PPT states of given ranks. We list some numerical results, and discuss how they may be understood in most cases by a simple counting of constraints, assuming the constraints to be independent.

We start with a useful exercise. We want to compute the real (as opposed to complex) dimension of the set of all r dimensional subspaces of an N dimensional complex Hilbert space.

First note that the unitary group $\mathrm{U}(k)$ has k^2 real dimensions. Take an orthonormal basis of the Hilbert space. The first r basis vectors define an r dimensional subspace, the orthogonal complement of which is defined by the last $s = N - r$ basis vectors. A $\mathrm{U}(N)$ transformation transforms this basis into another orthonormal basis, but the $\mathrm{U}(r)$ transformations within the first r basis vectors, and the $\mathrm{U}(s)$ transfomations within the last s basis vectors, do not change either subspace. It follows that the dimension of the set of r dimensional subspaces, equal to the dimension of the set of s dimensional subspaces, is

$$d = N^2 - r^2 - s^2 = 2rs \; . \tag{96}$$

Assuming that we have found a PPT state ρ of rank (m, n), it lies on a surface of rank (m, n) PPT states. We compute the dimension of the surface at this point by counting the number of independent solutions A of eq. (35),

$$(\mathbf{Q} + \widetilde{\mathbf{Q}})A = 0 \; , \tag{97}$$

equivalent to the two equations

$$\mathbf{Q}A = QAQ = 0 \; , \qquad \widetilde{\mathbf{Q}}A = (\widetilde{Q}A^P\widetilde{Q})^P = 0 \; . \tag{98}$$

We have to throw away the trivial solution $A = \rho$. We get a lower bound for the dimension if we assume that the constraints on A from the two equations in eq. (98) are independent. The equation $QAQ = 0$ represents $(N - m)^2$ real constraints, since Q is the orthogonal projection on the $N - m$ dimensional subspace $\mathrm{Ker}\,\rho$. Similarly, the equation $\widetilde{Q}A^P\widetilde{Q} = 0$ represents $(N-n)^2$ real constraints, since $\widetilde{Q}$ is the orthogonal projection on the $N - n$ dimensional subspace $\mathrm{Ker}\,\rho^P$. Because the constraints are not necessarily independent, we get the following lower bound for the dimension,

$$d \geq N^2 - (N - m)^2 - (N - n)^2 - 1 \; . \tag{99}$$

Take $N = 3 \times 3 = 9$ as an example. We find numerically that eq. (99) holds with equality for all ranks from the full rank $(m, n) = (9, 9)$ down to $(m, n) = (5, 5)$. In particular, for rank $(5, 5)$ the dimension of the surface is

$$d = 9^2 - 4^2 - 4^2 - 1 = 48 \; . \tag{100}$$

By eq. (96) the set of 5 dimensional subspaces has dimension 40, hence we should expect to find an 8 dimensional surface of rank $(5, 5)$ PPT states in every 5 dimensional subspace. And that is actually what we find.

For rank $(4, 4)$ the constraints are not all independent, and we have the strict inequality

$$d = 36 > 9^2 - 5^2 - 5^2 - 1 = 30 \; . \tag{101}$$

The set of 4 dimensional subspaces has again dimension 40, hence there can not exist rank $(4, 4)$ PPT states in every 4 dimensional subspace. There are $40 - 36 = 4$ constraints restricting the 4 dimensional subspaces supporting rank $(4, 4)$ PPT states, and in each 4 dimensional subspace there can exist at most one unique such state. The 4 constraints are the conditions that the 4 parameters a, b, c, d in eq. (47), or p, q, r, s in eq. (50), have to be real.

If we want to compute the dimension of the surface of rank (m,n) PPT states with fixed image space, we have to count the independent solutions of eq. (36),

$$(\mathbf{I}-\mathbf{P}+\widetilde{\mathbf{Q}})A=0\ , \tag{102}$$

equivalent to the two equations

$$\mathbf{P}A=PAP=A\ ,\qquad \widetilde{\mathbf{Q}}A=(\widetilde{Q}A^P\widetilde{Q})^P=0\ . \tag{103}$$

The equation $\mathbf{P}A=A$ leaves m^2 real parameters in A and represents N^2-m^2 real constraints, as is visualized in eq. (17). The lower bound on the dimension is therefore

$$d\geq N^2-(N^2-m^2)-(N-n)^2-1=m^2-(N-n)^2-1\ . \tag{104}$$

In the above example with $N=9$ and $(m,n)=(5,5)$ we find numerically $d=8$, as already mentioned, so that the inequality in eq. (104) holds as an equality. With $(m,n)=(4,4)$, on the other hand, we get

$$d=0\geq 4^2-5^2-1=-10\ . \tag{105}$$

9 Numerical integration

In this section we will describe a numerical method for tracing curves on a surface of PPT states of fixed ranks (m,n). This is a tool for studying the geometry of the surface, for example by tracing geodesics to see how they curve, or studying how the surface approaches a boundary consisting of states of lower ranks.

9.1 Equations of motion

The perturbation expansion $\rho(t+\epsilon)=\rho(t)+\epsilon A$ for $\rho=\rho(t)$ is equivalent to the differential equation

$$\dot{\rho}=A\ . \tag{106}$$

We use the notation

$$\dot{\rho}=\frac{\mathrm{d}\rho}{\mathrm{d}t}\ ,\qquad \dot{\rho}^+=\frac{\mathrm{d}\rho^+}{\mathrm{d}t}\ . \tag{107}$$

We defined the pseudoinverse ρ^+ in eq. (4), in order to define $P=\rho^+\rho=\rho\rho^+$ and $Q=\mathbb{1}-P$, the orthogonal projections on $\mathrm{Img}\,\rho$ and $\mathrm{Ker}\,\rho$, respectively. There are similar relations for $\widetilde{P}$, the projection on $\mathrm{Img}\,\rho^P$, and $\widetilde{Q}=\mathbb{1}-\widetilde{P}$, the projection on $\mathrm{Ker}\,\rho^P$. We defined orthogonal projections on H_N, the space of Hermitean matrices, in eq. (13) and eq. (32).

If X is a Hermitean matrix with $\mathrm{Img}\,X\subset\mathrm{Img}\,\rho$ then $X=PX=XP$, or equivalently, $QX=XQ=0$. Assuming that these relations hold at any "time" t we may differentiate and get that

$$\dot{X}=\dot{P}X+P\dot{X}=\dot{X}P+X\dot{P}\ . \tag{108}$$

Equivalently,

$$Q\dot{X}=\dot{P}X\ ,\qquad \dot{X}Q=X\dot{P}\ . \tag{109}$$

Multiplication by Q from the left and from the right gives that

$$Q\dot{X}Q = 0 \ . \tag{110}$$

It follows further that

$$\dot{X} = (P+Q)\dot{X}(P+Q) = P\dot{X}P + X\dot{P} + \dot{P}X \ . \tag{111}$$

The special case $X = \rho$ gives the equation

$$QAQ = 0 \tag{112}$$

as a consistency condition for eq. (106) with the relations $\rho = P\rho = \rho P$. Eq. (112) is the same as eq. (11), the condition for the rank of ρ to be constant. We may want to replace it with the stronger condition that Img ρ should be constant, eq. (9),

$$PAP = A \ . \tag{113}$$

Setting $X = \rho$ in eq. (109) gives the equations

$$QA = \dot{P}\rho \ , \qquad AQ = \rho\dot{P} \ , \tag{114}$$

and multiplication by ρ^+ gives that

$$QA\rho^+ = \dot{P}P \ , \qquad \rho^+ AQ = P\dot{P} \ . \tag{115}$$

Differentiating the equation $P = P^2$ gives that $\dot{P} = \dot{P}P + P\dot{P}$, hence

$$\dot{P} = QA\rho^+ + \rho^+ AQ \ . \tag{116}$$

Differentiating the relation $\rho^+ = \rho^+\rho\rho^+$ we get that

$$\dot{\rho}^+ = \dot{\rho}^+ P + \rho^+ A\rho^+ + P\dot{\rho}^+ \ . \tag{117}$$

When we left and right multiply here by P we obtain the relation

$$P\dot{\rho}^+ P = -\rho^+ A\rho^+ \ . \tag{118}$$

Hence, using eq. (111) with $X = \rho^+$, together with eq. (116), we get that

$$\dot{\rho}^+ = QA(\rho^+)^2 + (\rho^+)^2 AQ - \rho^+ A\rho^+ \ . \tag{119}$$

The equations (106), (116), and (119) may be integrated together, as soon as we specify how to calculate A as a function of ρ. There are, of course, equations similar to (116) and (119) that hold for the projection $\widetilde{P}$ related to the partial transpose ρ^P, and for the pseudoinverse $(\rho^P)^+$.

As a specific example, consider how to generate a curve $\rho = \rho(t)$ lying on the 48 dimensional surface in H_N of rank $(5,5)$ PPT states in 3×3 dimensions passing through a given state $\rho(0)$. We then have to satisfy the two conditions on A that

$$\mathbf{Q}A = QAQ = 0 \ , \qquad \widetilde{\mathbf{Q}}A = (\widetilde{Q}A^P\widetilde{Q})^P = 0 \ . \tag{120}$$

Or equivalently eq. (35),

$$(\mathbf{Q} + \widetilde{\mathbf{Q}})A = 0 \ . \tag{121}$$

Alternatively, we may want to generate a curve that follows the 8 dimensional surface in H_N of rank $(5,5)$ PPT states such that the 5 dimensional subspace Img ρ is kept fixed, but the 5 dimensional subspace Img ρ^P is allowed to change. This means that we replace the condition $QAQ = 0$ by the condition $PAP = A$. The single condition to be satisfied is then eq. (36),

$$(\mathbf{I} - \mathbf{P} + \widetilde{\mathbf{Q}})A = 0 \ . \tag{122}$$

In this case P is constant but $\widetilde{Q} = \widetilde{Q}(t)$ may vary as a function of t.

9.2 Geodesic equations

Both conditions (121) and (122) are of the form

$$\mathbf{T}A = 0 \; . \tag{123}$$

Differentiating this equation gives that

$$\mathbf{T}\dot{A} + \dot{\mathbf{T}}A = 0 \; . \tag{124}$$

It follows that

$$\dot{A} = B - \mathbf{T}^{+}\dot{\mathbf{T}}A \; , \tag{125}$$

where $\mathbf{T}^{+}$ is the pseudoinverse of $\mathbf{T}$, and B is an arbitrary Hermitean matrix with $\mathbf{T}B = 0$.

By definition, a geodesic on an embedded surface (think of a great circle on the surface of a sphere as an example) is a curve which does not change its direction on the surface. Hence, it changes direction in the embedding space only as much as it has to in order to stay on the surface. This would mean that we choose $B = 0$ in eq. (125). Or if we normalize A to unit length, fixing $\mathrm{Tr}\, A^2 = 1$, we set $B = \alpha A$ and choose α such that $\mathrm{Tr}(\dot{A}A) = 0$.

9.3 Numerical results

We have done numerical integrations by a standard fourth order Runge–Kutta method. With ρ and A of order one and time steps of order 10^{-4} this gives a precision of order 10^{-16}, which is the machine precision.

Figure 3 shows a geodesic curve $\rho(t)$ on the 8 dimensional curved surface of rank $(5,5)$ PPT states with $\mathrm{Img}\,\rho(t)$ constant. Figure 4 shows the 5 nonzero eigenvalues of ρ and ρ^P. The condition that one eigenvalue of either ρ or ρ^P goes to zero defines the boundary of the surface. We see that the curve approaches the boundary twice, but turns around each time and continues in the interior. The eigenvalue spectra of ρ and ρ^P are remarkably similar, yet they are not identical. When both ρ and ρ^P simultaneously get one dominant eigenvalue, we interpret it as an indication that ρ approaches a pure product state.

It is quite natural that a geodesic chosen at random will not hit the boundary, since the boundary consists of rank $(4,4)$ PPT states and has dimension 4, while the surface itself has dimension 8. In order to hit the boundary we can not follow a geodesic, we have to integrate the equation $\dot{\rho} = A$ and choose the direction A in such a way that the smallest positive eigenvalue of ρ goes to zero. When we do so, the smallest eigenvalue of ρ^P goes to zero simultaneously with the eigenvalue of ρ, although the ratio between the two eigenvalues goes to a value different from one. Hence the curve ends at a $(4,4)$ state on the boundary. The explanation for this coupling of eigenvalues of ρ and ρ^P was given in Subsection 6.2.

10 Summary

The work presented here is part of an ongoing programme to study quantum entanglement in mixed states. We have studied here low rank entangled PPT states using perturbation theory and the close relation between PPT states and product vectors.

One result obtained is an understanding of how to construct rank $(5,5)$ PPT states in 3×3 dimensions by perturbing rank $(4,4)$ states. We use perturbation theory to study surfaces of PPT states

of given ranks, and in particular to compute dimensions of such surfaces, for example the surface of $(5, 5)$ states. However, it is still an unsolved problem how to construct general rank $(5, 5)$ PPT states that are not close to rank $(4, 4)$ states. We are even farther from a full understanding of higher rank PPT states in 3×3 dimensions, or in higher dimensions.

A special class of PPT states are those of special ranks so that their kernel is spanned by product vectors and contains a finite number of product vectors. We have shown that these states may be reconstructed uniquely from a subset of the product vectors in the kernel, and the number of product vectors needed may be smaller than the dimension of the kernel. This result raises new interesting questions to be answered by future research, for example, how to identify finite sets of product vectors that define PPT states with these product vectors in their kernel.

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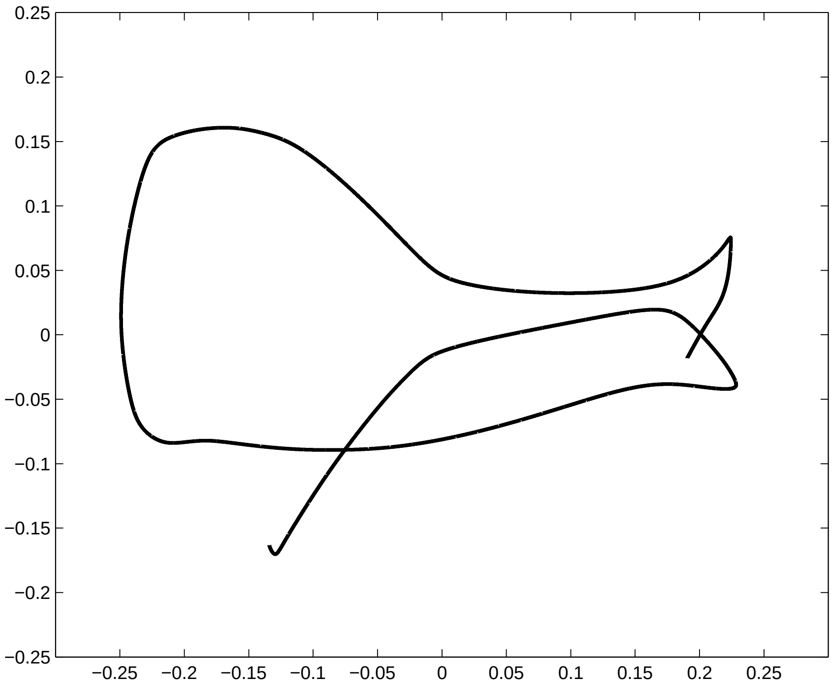

Figure 3: A projection of a geodesic curve on the 8 dimensional surface of rank $(5, 5)$ PPT states with a fixed image space. We have made a principal component analysis and plotted the two largest principal components. The curve starts middle right and ends lower left.

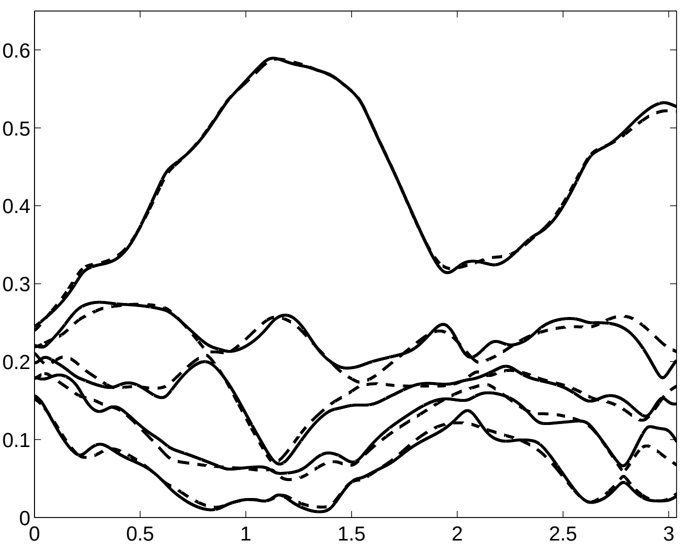

Figure 4: Variation along the curve in Fig. 3 of the 5 nonzero eigenvalues of the density matrix (full drawn lines) and its partial transpose (broken lines). The abscissa is the arc length along the curve.

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